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Scattering and reaction cross sections of $e^{\pm}-Ps$ system are calculated for total angular momentum $L=0,1$ and 2 and energies between the $Ps(n=2)-Ps(n=3)$ threshold. We solved a set of Faddeev-Merkuriev and Lippmann-Schwinger integral equations by applying the Coulomb-Sturmian separable expansion technique. We found that the excited positronium states play dominating roles in scattering processes.

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The $e^{\pm}-Ps$ system plays a very important role in studying the antimatter. While, on the experimental side, new experiments, that involve the positronium in one way or another, are being carried out or planned [1], on the theoretical side, the existing calculations are restricted for low energy elastic scattering below the $Ps(n=2)$ threshold (see Ref. [2] and references therein).

Recently, based on a three-potential picture, we have developed a new method for treating three-body Coulombic systems [3]. The three-potential formalism results in a set of Faddeev-Merkuriev and Lippmann-Schwinger integral equations. These integral equations were solved by the Coulomb-Sturmian separable expansion technique.

In this paper we present scattering and reaction calculations for energies between the $Ps(n=2)-Ps(n=3)$ threshold and for total angular momentum $L=0,1,$ and 2. First we outline the method of Ref. [3] to the $e^{\pm}-Ps$ system and then present the results.

In the $e^{\pm}-Ps$ system two particles are always identical. Let us denote them by 1 and 2, and the non-identical one by 3. The Hamiltonian is given by

$$H=H^0+v_1^C+v_2^C+v_3^C, \tag{1}$$

where H^0 is the three-body kinetic energy operator and v_α^C denotes the Coulomb interaction in the subsystem α. We use the usual configuration-space Jacobi coordinates x_α and y_α; x_α is the coordinate between the pair (β,γ) and y_α is the coordinate between the particle α and the center of mass of the pair (β,γ). Thus the potential v_α^C, the interaction of the pair (β,γ), appears as $v_\alpha^C(x_\alpha)$. We also use the notation $X=\{x_\alpha,y_\alpha\}\in\mathbf{R}^6$.

The Hamiltonian (1) is defined in the three-body Hilbert space. So, the two-body potential operators are formally embedded in the three-body Hilbert space,

$$v^C=v^C(x)\mathbf{1}_y, \tag{2}$$

where $\mathbf{1}_y$ is a unit operator in the two-body Hilbert space associated with the y coordinate. The role of a Coulomb potential in a three-body Coulombic system is twofold. In one hand, it acts like a long-range potential since it modifies the asymptotic motion. On the other hand, however, it acts like a short-range potential, since it correlates strongly the particles and may support bound states. Merkuriev introduced a separation of the three-body configuration space into different asymptotic regions [4]. The two-body asymptotic region Ω is defined as a part of the three-body configuration space where the conditions

$$|x|<x_0(1+|y|/y_0)^{1/\nu}, \tag{3}$$

with $x_0,y_0>0$ and $\nu>2$, are satisfied. Merkuriev proposed to split the Coulomb interaction in the three-body configuration space into short-range and long-range terms

$$v^C=v^{(s)}+v^{(l)}, \tag{4}$$

where the superscripts s and l indicate the short- and long-range attributes, respectively. The splitting is carried out with the help of a splitting function ζ,

$$v^{(s)}(x,y)=v^C(x)\zeta(x,y), \tag{5}$$
$$v^{(l)}(x,y)=v^C(x)[1-\zeta(x,y)]. \tag{6}$$

The function ζ is defined such that

$$\zeta(x,y)\xrightarrow{X\to\infty}\begin{cases}1, & X\in\Omega\\ 0 & \text{otherwise.}\end{cases} \tag{7}$$

In practice usually the functional form

$$\zeta(x,y)=2/\left\{1+\exp\left[(x/x^0)^\nu/(1+y/y^0)\right]\right\}, \tag{8}$$

is used.

In the Hamiltonian (1) the potential v_3^C, acting between the identical particles, is a repulsive Coulomb potential which does not support bound states. Consequently, the entire v_3^C can be considered as long-range potential. Then, the long-range Hamiltonian is defined as

$$H^{(l)}=H^0+v_1^{(l)}+v_2^{(l)}+v_3^C, \tag{9}$$

and the three-body Hamiltonian takes the form

$$H = H^{(l)} + v_1^{(s)} + v_2^{(s)}. \tag{10}$$

So, the Hamiltonian of the $e^{\pm} - Ps$ system appears formally as a three-body Hamiltonian with two short-range potentials. The Faddeev procedure is applicable, and, in this case, we get a set of two-component Faddeev-Merkuriev integral equations

$$|\psi_1\rangle = |\Phi_1^{(l)}\rangle + G_1^{(l)} v_1^{(s)} |\psi_2\rangle \tag{11}$$

$$|\psi_2\rangle = G_2^{(l)} v_2^{(s)} |\psi_1\rangle, \tag{12}$$

where $|\phi_\alpha^{(l)}\rangle$ and $G_\alpha^{(l)}$ are eigenstate and resolvent operator, respectively, of the channel Coulomb Hamiltonian

$$H_\alpha^{(l)} = H^{(l)} + v_\alpha^{(s)}. \tag{13}$$

Since the particles 1 and 2 are identical the Faddeev components $|\psi_1\rangle$ and $|\psi_2\rangle$, in their own natural Jacobi coordinates, have the same functional forms

$$\langle x_1 y_1 | \psi_1 \rangle = \langle x_2 y_2 | \psi_2 \rangle = \langle xy | \psi \rangle. \tag{14}$$

Therefore we can determine $|\psi\rangle$ from the first equation only

$$|\psi\rangle = |\Phi_1^{(l)}\rangle + G_1^{(l)} v_1^{(s)} p\mathcal{P} |\psi\rangle, \tag{15}$$

where $\mathcal{P}$ is the operator for the permutation of indexes 1 and 2 and $p = \pm 1$ are eigenvalues of $\mathcal{P}$. We note that although this integral equation has only one component yet gives full account on the asymptotic and symmetry properties of the system.

We solve this integral equation by using the Coulomb–Sturmian separable expansion approach. The Coulomb-Sturmian (CS) functions are defined by

$$\langle r | nl \rangle = \left[\frac{n!}{(n+2l+1)!} \right]^{1/2} (2br)^{l+1} \exp(-br) L_n^{2l+1}(2br), \tag{16}$$

with n and l being the radial and orbital angular momentum quantum numbers, respectively, and b is the size parameter of the basis. The CS functions $\{|nl\rangle\}$ form a biorthonormal discrete basis in the radial two-body Hilbert space; the biorthogonal partner defined by $\langle r|\widetilde{nl}\rangle = \langle r|nl\rangle / r$.

Since the three-body Hilbert space is a direct product of two-body Hilbert spaces an appropriate basis can be defined as the angular momentum coupled direct product of the two-body bases

$$|n\nu l\lambda\rangle_\alpha = |nl\rangle_\alpha \otimes |\nu\lambda\rangle_\alpha, \quad (n, \nu = 0, 1, 2, \dots), \tag{17}$$

where $|nl\rangle_\alpha$ and $|\nu\lambda\rangle_\alpha$ are associated with the coordinates x_α and y_α, respectively. With this basis the completeness relation takes the form (with angular momentum summation implicitly included)

$$\mathbf{1} = \lim_{N\to\infty} \sum_{n,\nu=0}^{N} |\widetilde{n\nu l\lambda}\rangle_\alpha \, {}_\alpha\langle n\nu l\lambda| = \lim_{N\to\infty} \mathbf{1}_\alpha^N, \tag{18}$$

where $\langle xy|\widetilde{n\nu l\lambda}\rangle = \langle xy|n\nu l\lambda\rangle/(xy)$.

We make the following approximation on the integral equation (15)

$$|\psi\rangle = |\Phi_1^{(l)}\rangle + G_1^{(l)} \mathbf{1}_1^N v_1^{(s)} p\mathcal{P} \mathbf{1}_1^N |\psi\rangle, \tag{19}$$

i.e. the operator $v_1^{(s)} p\mathcal{P}$ is approximated in the three-body Hilbert space by a separable form, viz.

$$\begin{aligned} v_1^{(s)} p\mathcal{P} &= \lim_{N\to\infty} \mathbf{1}_1^N v_1^{(s)} p\mathcal{P} \mathbf{1}_1^N \\ &\approx \mathbf{1}_1^N v_1^{(s)} p\mathcal{P} \mathbf{1}_1^N \\ &\approx \sum_{n,\nu,n',\nu'=0}^{N} |\widetilde{n\nu l\lambda}\rangle_1 \, \underline{v}_1^{(s)} \, {}_1\langle \widetilde{n'\nu' l'\lambda'}|, \end{aligned} \tag{20}$$

where $\underline{v}_1^{(s)} = {}_1\langle n\nu l\lambda | v_1^{(s)} p\mathcal{P} | n'\nu' l'\lambda'\rangle_1$. Utilizing the properties of the exchange operator $\mathcal{P}$ these matrix elements can be written in the form $\underline{v}_1^{(s)} = p \times {}_1\langle n\nu l\lambda | v_1^{(s)} | n'\nu' l'\lambda'\rangle_2$, and can be evaluated numerically by using the transformation of the Jacobi coordinates.

Now, with this approximation, the solution of the inhomogeneous Faddeev-Merkuriev equation turns into a solution of a matrix equation for the component vector $\underline{\psi} = {}_1\langle \widetilde{n\nu l\lambda} | \psi \rangle$

$$\underline{\psi} = \underline{\Phi}_1^{(l)} + \underline{G}_1^{(l)} \underline{v}_1^{(s)} \underline{\psi} \tag{21}$$

where

$$\underline{\Phi}_1^{(l)} = {}_1\langle \widetilde{n\nu l\lambda} | \Phi_1^{(l)} \rangle \tag{22}$$

and

$$\underline{G}_1^{(l)} = {}_1\langle \widetilde{n\nu l\lambda} | G_1^{(l)} | \widetilde{n'\nu' l'\lambda'} \rangle_1. \tag{23}$$

The formal solution of Eq. (21) is given by

$$[(\underline{G}_1^{(l)})^{-1} - \underline{v}_1^{(s)}] \underline{\psi} = (\underline{G}_1^{(l)})^{-1} \underline{\Phi}_1^{(l)}. \tag{24}$$

Unfortunately neither $\underline{G}_1^{(l)}$ nor $\underline{\Phi}_1^{(l)}$ are known. They are related to the Hamiltonian $H_1^{(l)}$, which itself is a complicated three-body Coulomb Hamiltonian. In the three-potential formalism [3] $\underline{G}_1^{(l)}$ is linked to simpler quantities via solution of a Lippmann-Schwinger equation,

$$(\underline{G}_1^{(l)})^{-1} = (\underline{\widetilde{G}}_1)^{-1} - \underline{U}^1, \tag{25}$$

where

$$\underline{\widetilde{G}}_{1\,{}_{n\nu l\lambda, n'\nu' l'\lambda'}} = {}_1\langle \widetilde{n\nu l\lambda} | \widetilde{G}_1 | \widetilde{n'\nu' l'\lambda'} \rangle_1 \tag{26}$$

and

$$\underline{U}^1_{n\nu l\lambda,n'\nu'l'\lambda'} = {}_1\langle n\nu l\lambda|U^1|n'\nu'l'\lambda'\rangle_1. \quad (27)$$

The operator $\widetilde{G}_1$ is the resolvent operator of the Hamiltonian

$$\widetilde{H}_1 = H^0 + v_1^C. \quad (28)$$

The polarization potential U^1 is defined by

$$U^1 = v_2^{(l)} + v_3^C, \quad (29)$$

and its matrix elements can again be evaluated numerically.

Similarly, also $\underline{\Phi}_1^{(l)}$ can be linked to simpler quantities

$$[(\underline{\widetilde{G}}_1)^{-1} - \underline{U}^1]\underline{\Phi}_1^{(l)} = (\underline{\widetilde{G}}_1)^{-1}\underline{\widetilde{\Phi}}_1, \quad (30)$$

where $\underline{\widetilde{\Phi}}_{1_{n\nu l\lambda}} = {}_1\langle\widetilde{n\nu l\lambda}|\widetilde{\Phi}_1\rangle$, and $\widetilde{\Phi}_1$ is eigenstate of $\widetilde{H}_1$.

The three-particle free Hamiltonian can be written as a sum of two-particle free Hamiltonians

$$H^0 = h^0_{x_1} + h^0_{y_1}. \quad (31)$$

Consequently the Hamiltonian $\widetilde{H}_1$ of Eq. (28) appears as a sum of two Hamiltonians acting on different coordinates

$$\widetilde{H}_1 = h_{x_1} + h_{y_1}, \quad (32)$$

with $h_{x_1} = h^0_{x_1} + v_1^C(x_1)$ and $h_{y_1} = h^0_{y_1}$, which, of course, commute. Therefore its eigenstate, in CS representation, appears as

$${}_1\langle\widetilde{n\nu l\lambda}|\widetilde{\Phi}_1\rangle = {}_1\langle\widetilde{nl}|\phi_1\rangle \times {}_1\langle\widetilde{\nu\lambda}|\chi_1\rangle, \quad (33)$$

where $|\phi_1\rangle$ and $|\chi_1\rangle$ are bound and scattering eigenstates of h_{x_1} and h_{y_1}, respectively.

The matrix elements of $\widetilde{G}_1$ can be determined by making use of the convolution theorem

$$\underline{\widetilde{G}}_1(z) = \frac{1}{2\pi\mathrm{i}}\oint_C dz'\, \underline{g}_{x_1}(z-z')\, \underline{g}_{y_1}(z'), \quad (34)$$

where g_{x_1} and g_{y_1} are resolvent operators of h_{x_1} and h_{y_1}, respectively. The corresponding CS matrix elements of the two-body Green's operators for all complex energies and of the two-body solutions in Eq. (33) are known analytically. The contour C should encircle, in positive direction, the spectrum of h_{y_1} without penetrating into the spectrum of h_{x_1}. Further details on the contour and on those CS matrix elements are given in Ref. [3] and references therein.

The S-matrix of the $e^\pm - Ps$ scattering process, in the three-potential picture [3], can be decomposed as

$$S^{(2)}_{fi} = -2\pi\mathrm{i}\delta(E_f - E_i) \times(\langle\widetilde{\Phi}^{(-)}_{1f}|U^1|\Phi^{(l)(+)}_{1i}\rangle + \langle\Phi^{(l)(-)}_{1f}|v_1^{(s)}|\psi^{(+)}_{2i}\rangle), \quad (35)$$

where i and f refer to the initial and the final states, respectively. Having the solutions $\underline{\psi}$ and $\underline{\Phi}^{(l)}$ the matrix elements can easily be evaluated.

In the numerical calculations we used atomic units. For the parameters of the splitting function (8) we took $x_0 = 10$, $y_0 = 20$ and $\nu = 2.1$, respectively, and for the size parameter of the CS basis we used $b = 0.2$. In the expansion of the potentials we went up to 11 angular momentum channels and, in each angular momentum channels, up to $N = 27$ CS functions. This way we achieved convergence up to $2-3\%$ and also the K-matrix were symmetric with a similar accuracy. Some of the results were cross-checked by the results of configuration-space differential equation calculation [5], and we found again very good agreements.

The results for total angular momentum $L = 0$, $L = 1$ and $L = 2$ are given in Tables I, II and III, respectively. We can see that the excited positronium states play dominating roles in scattering processes, especially when the total energies approach the positronium excitation threshold (from above). This behavior is consistent with the rather large size of the excited positronium targets, where the long-range polarization potential play dominant roles. This behavior is similar to the phenomena found in $\bar{p} - \mathrm{Ps}$ multichannel scattering process, where this mechanism dominates the antihydrogen formation cross section (will be published in a separate paper).

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TABLE I. $L = 0$ partial cross sections (in πa_0^2) in the $Ps(n=2) - Ps(n=3)$ gap. Channel numbers 1,2 and 3 denote the channels $e^\pm(\lambda=0) + Ps(1s)$, $e^\pm(\lambda=0) + Ps(2s)$ and $e^\pm(\lambda=1) + Ps(2p)$ respectively.

k_1	Ch.#	1	2	3
		$L=0 \quad p=1$		
	1	4.384	0.043	0.032
0.51	2	1.125	67.79	0.245
	3	0.851	0.247	301.6
	1	4.055	0.043	0.033
0.52	2	0.576	60.77	45.45
	3	0.445	45.51	62.48
	1	3.756	0.043	0.037
0.53	2	0.402	43.57	19.28
	3	0.349	19.32	63.77
	1	3.484	0.044	0.041
0.54	2	0.324	28.39	2.12
	3	0.286	2.13	71.74
		$L=0 \quad p=-1$		
	1	12.52	0.0001	0.0000
0.51	2	0.0023	121.69	0.941

	3	0.0011	0.936	263.84
	1	11.79	0.0001	0.0001
0.52	2	0.0021	102.42	35.32
	3	0.0009	35.28	42.75
	1	11.10	0.0002	0.0002
0.53	2	0.0025	36.60	31.33
	3	0.0019	31.28	37.06
	1	10.45	0.0003	0.0004
0.54	2	0.0020	8.93	19.78
	3	0.0025	19.75	44.23

TABLE II. $L = 1$ partial cross sections (in πa_0^2) in the $Ps(n = 2) - Ps(n = 3)$ gap. Channel numbers 1,2,3 and 4 denote the channels $e^{\pm}(\lambda = 1) + Ps(1s)$, $e^{\pm}(\lambda = 1) + Ps(2s)$, $e^{\pm}(\lambda = 0) + Ps(2p)$ and $e^{\pm}(\lambda = 2) + Ps(2p)$, respectively.

k_1	Ch.#	1	2	3	4
		$L = 1$	$p = 1$		
	1	20.22	0.090	0.466	0.246
0.51	2	2.378	296.76	30.16	29.21
	3	12.21	30.17	90.13	139.14
	4	6.49	29.40	138.90	591.54
	1	19.24	0.086	0.617	0.317
0.52	2	1.16	17.76	56.03	26.56
	3	8.33	55.91	127.26	66.25
	4	4.28	26.37	66.05	305.29
	1	18.32	0.095	0.804	0.398
0.53	2	0.874	65.19	50.25	38.59
	3	7.47	50.16	69.26	28.60
	4	3.69	38.38	28.52	174.53
	1	16.91	0.207	0.916	0.599
0.54	2	1.48	81.55	50.21	19.94
	3	6.50	50.12	66.48	10.43
	4	4.20	19.75	10.36	169.84
		$L = 1$	$p = -1$		
	1	12.80	0.458	0.184	0.175
0.51	2	12.16	290.22	44.19	9.62
	3	4.89	44.28	737.30	135.86
	4	4.66	9.63	135.60	813.33
	1	11.93	0.484	0.201	0.194
0.52	2	6.60	21.53	9.78	66.71
	3	2.71	9.77	246.08	46.32
	4	2.64	66.40	46.17	308.15
	1	11.14	0.514	0.229	0.214
0.53	2	4.82	81.03	9.85	79.18
	3	2.13	9.87	52.74	14.22
	4	2.01	78.89	14.16	94.31
	1	10.41	0.542	0.262	0.232
0.54	2	3.96	145.62	4.51	50.12
	3	1.91	4.52	3.24	4.66
	4	1.68	49.97	4.65	25.25

TABLE III. $L = 2$ partial cross sections (in πa_0^2) in the $Ps(n = 2) - Ps(n = 3)$ gap. Channel numbers 1,2,3 and 4 denote the channels $e^{\pm}(\lambda = 2) + Ps(1s)$, $e^{\pm}(\lambda = 2) + Ps(2s)$, $e^{\pm}(\lambda = 1) + Ps(2p)$ and $e^{\pm}(\lambda = 3) + Ps(2p)$, respectively.

k_1	Ch.#	1	2	3	4
		$L = 1$	$p = 1$		
	1	7.78	0.010	0.005	0.004
0.51	2	0.236	917.53	174.78	64.21
	3	0.113	175.24	873.28	203.44
	4	0.097	63.72	203.03	888.39
	1	7.58	0.025	0.004	0.012
0.52	2	0.333	227.40	28.16	78.54
	3	0.046	28.16	773.01	69.57
	4	0.153	76.55	69.05	428.25
	1	7.38	0.048	0.003	0.025
0.53	2	0.438	68.33	10.13	92.31
	3	0.026	10.02	502.06	30.49
	4	0.217	89.59	30.02	231.33
	1	7.18	0.081	0.003	0.046
0.54	2	0.558	40.57	6.30	90.67
	3	0.028	6.29	307.42	15.42
	4	0.311	88.17	15.02	127.53
		$L = 1$	$p = -1$		
	1	6.61	0.025	0.037	0.026
0.51	2	0.644	941.82	194.33	36.50
	3	0.950	196.67	79.94	58.60
	4	0.656	35.57	57.09	1080.61
	1	6.40	0.040	0.092	0.054
0.52	2	0.546	427.67	3.46	16.52
	3	1.22	3.29	293.60	0.754
	4	0.728	15.06	0.860	510.53
	1	6.18	0.050	0.135	0.078
0.53	2	0.465	159.41	37.79	20.14
	3	1.22	37.34	325.85	7.27
	4	0.711	18.57	7.22	314.93
	1	5.95	0.055	0.221	0.112
0.54	2	0.386	72.91	49.02	22.41
	3	1.55	48.23	256.51	11.45
	4	0.757	21.33	11.44	210.85

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